

A DUALITY-BASED OPTIMIZATION APPROACH FOR MODEL ADAPTIVITY IN HETEROGENEOUS MULTISCALE PROBLEMS

MATTHIAS MAIER* AND ROLF RANNACHER†

Abstract. This paper introduces a novel framework for model adaptivity in the context of heterogeneous multiscale problems. The framework is based on the idea to interpret model adaptivity as a *minimization problem* of local error indicators, that are derived in the general context of the *Dual Weighted Residual* (DWR) method. Based on the optimization approach a post-processing strategy is formulated that lifts the requirement of strict a priori knowledge about applicability and quality of effective models. This allows for the systematic, “goal-oriented” tuning of *effective models* with respect to a *quantity of interest*. The framework is tested numerically on elliptic diffusion problems with different types of heterogeneous, random coefficients, as well as an advection-diffusion problem with strong microscopic, random advection field.

Key words. finite element method, mesh adaptation, model optimization, model adaptation, goal-oriented adaptivity, DWR method

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1. Introduction. A number of different approaches for modeling multiscale phenomena in the context of finite-element methods have been introduced over the last years. They either rely on the existence of a periodic or stochastic substructure or on the scale-dependent splitting of variational solution- and test spaces [7, 9, 10, 13]. The use of multiscale methods comes at a significant price with respect to sources of error: Among the usual discretization error due to a numerical approximation of the partial differential equation (PDE), multiscale methods exhibit an inherent *model error* resulting from a *modeling assumption* for scale separation. This makes the idea of a posteriori error estimation, where a quantitative estimate for the different sources of error is computed by means of a post-processing approach highly attractive. The a posteriori control of discretization errors for multiscale methods is well understood [1, 11, 12, 14, 15].

The novelty of a posteriori error estimation with respect to multiscale methods lies in the possibility for *model adaptivity*. First results for *estimating and controlling the model error* in the context of multiscale schemes were given by Oden et al. [19–21] and Braack and Ern [6] in the context of the *Heterogeneous Multiscale Method* (HMM) [9]. The key idea is to use the error-identity stemming from the *Dual Weighted Residual* (DWR) method introduced by Becker and Rannacher [4, 5] to quantify a local model error. This information can then be used for different model-adaptation strategies: A possible approach is to locally switch from a cheap, coarse model to an expensive, full model within an adaptation cycle [6]. Alternatively, as a pure post-processing strategy, *region of influence* can be constructed on which a finescale correction is computed in full [19–21].

Based on a multiscale framework introduced in a previous publications by the authors [16, 17], this paper presents a novel approach for model adaptivity. Instead of using an a priori choice of increasingly accurate models to switch between them (depending on the local error estimate), it uses the error identity obtained by the

*School of Mathematics, University of Minnesota, 206 Church Street SE, Minneapolis, MN 55455, USA. msmaier@umn.edu.

†Institute of Applied Mathematics, Heidelberg University, Im Neuenheimer Feld 205, 69120 Heidelberg, Germany. rannacher@iwr.uni-heidelberg

duality argument directly in a minimization problem. This has the advantage that no a priori knowledge about effective models and reconstruction principles has to be available. The optimization problem itself is used to select the optimal model.

The optimization approach requires a certain quality of the approximation of the dual solution that will be addressed with an efficient local reconstruction approach. The error identity lifts the question of suitable approximation in terms of a *quantity of interest* to the question of suitable approximation properties of the localization technique for the dual problem. The latter is typically measured in the L^2 -norm of the gradient of the error of the dual approximation, for which—depending on the localization approach—strong approximation properties are available. Thus, the proposed optimization framework can be interpreted as a multiscale method in its own right, where a reconstruction process is used for the dual solution. The *modeling aspect* of the optimization problem lies in the choice of the quantity of interest and the choice of local reconstruction of the dual solution.

The outline of the paper is as follows. In Section 2 an abstract multiscale scheme for model adaptation is outlined shortly [16, 17]. The section also covers the necessary a posteriori error analysis with the DWR method and an efficient approximation strategy for the solution of the dual problem involved. With this prerequisites at hand, a model-optimization framework is introduced in Section 3. It is based on a minimization problem formulated with the help of an error identity from the a posteriori error analysis. Implementational details are discussed in Section 4. In Section 5 an extensive numerical study for an elliptic diffusion problem and an advection-diffusion problem is shown. A conclusion and outlook is given in Section 6.

2. An abstract multiscale scheme for model adaptation. The discussion in this section is based on a multiscale scheme for model adaptation introduced by the authors [16, 17] that explicitly decouples all discretization and modeling parameters. It is a reformulation of the classical HMM method by E and Engquist [9] and shares similarities with model adaptation frameworks introduced by Oden and Vemaganti [19, 20] and Braack and Ern [6]. We briefly discuss a slightly simplified variant in this section. For a detailed introduction we refer to the aforementioned publications.

Let us consider the following multi-scale model problem: Find $u^\varepsilon \in H_0^1(\Omega)$ s. t.

$$(2.1) \quad (A^\varepsilon \nabla u^\varepsilon, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega),$$

on a bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) where the generally tensor-valued function $A^\varepsilon \in L^\infty(\Omega)^{d \times d}$ is of heterogeneous character and highly oscillating on a small length scale indicated by a scaling parameter ε . Here, $H_0^1(\Omega)$ is the usual first-order Sobolev Hilbert space with zero Dirichlet data along the boundary $\partial\Omega$. (\cdot, \cdot) denotes the L^2 scalar product on Ω and $\|\cdot\| = (\cdot, \cdot)^{1/2}$ the corresponding norm. The norms of other function spaces are indicated by subscripts, e. g., $\|\cdot\|_{L^\infty(\Omega)}$ or $\|\cdot\|_K = \|\cdot\|_{L^2(K)}$ for a subset $K \subset \Omega$. We assume the coefficient tensor A^ε to be symmetric and positive definite (uniformly in ε),

$$(2.2) \quad A_{ij}^\varepsilon = A_{ji}^\varepsilon, \quad \alpha |\xi|^2 \leq \sum_{i,j=1}^d A_{ij}^\varepsilon \xi_i \xi_j \leq \beta |\xi|^2, \quad \text{a. e. on } \Omega, \quad \xi \in \mathbb{R}^d,$$

with constants $\alpha, \beta \in \mathbb{R}_+$, so that (2.1) admits a unique solution.

Due to the finescale character of A^ε , a direct numerical simulation of (2.1) is computationally very expensive. We thus introduce an *effective model problem*

$$(2.3) \quad (A^\delta \nabla u^\delta, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega)$$

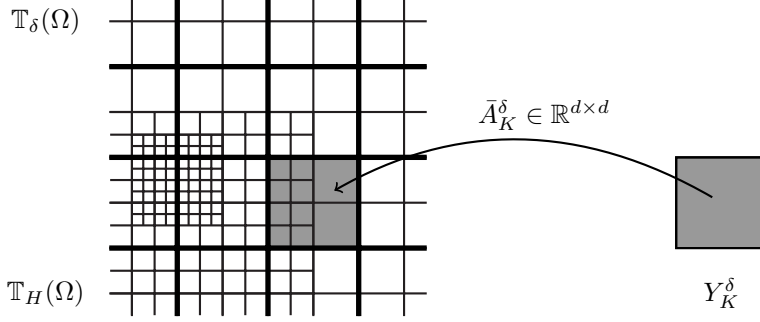


Figure 1: The computational domain Ω together with the *sampling mesh* $\mathbb{T}_\delta(\Omega)$ consisting of sampling regions $K \in \mathbb{T}_\delta$. The coarse mesh $\mathbb{T}_H(\Omega)$ used for the final finite-element discretization is a refinement of the sampling mesh \mathbb{T}_δ .

based on a sampling mesh $\mathbb{T}_\delta(\Omega)$ of Ω together with an effective tensor

$$(2.4) \quad \bar{A}^\delta : \mathbb{T}_\delta(\Omega) \rightarrow \mathbb{R}^{d \times d}$$

with region-wise constant values; see Figure 1.

REMARK 2.1. *Effective parameters $(\mathbb{T}_\delta(\Omega), A^\delta)$ can be obtained by different means, e. g., by using cell problems derived within a corresponding homogenization theory [2, 8]:*

$$(2.5) \quad \bar{A}_{ij}^\delta(K) := \oint_{Y_K^\delta} A^\varepsilon(x) (\nabla_x \omega_i(x) + \mathbf{e}_i) \cdot (\nabla_x \omega_j(x) + \mathbf{e}_j) \, dx,$$

where the $\omega_i \in \tilde{H}_{per}^1(Y_K^\delta)$ are solutions of a so-called cell problem

$$(2.6) \quad \int_{Y_K^\delta} A^\varepsilon(x) (\nabla_x \omega_i(x) + \mathbf{e}_i) \cdot \nabla \varphi = 0 \quad \forall \varphi \in \tilde{H}_{per}^1(Y_K^\delta),$$

or by using simple averaging strategies such as the geometric mean value [23]:

$$(2.7) \quad \log \bar{A}_{ij}^\delta(K) := \frac{1}{|Y_K^\delta|} \int_{Y_K^\delta} (\log A_{ij}^\varepsilon(y)) \, dy.$$

Here, Y_K^δ denotes a rescaled copy of the unit cell $Y = [0, 1]^d$ centered at the midpoint of a given sampling-mesh cell $K \in \mathbb{T}_\delta(\Omega)$. $\tilde{H}_{per}^1(Y_K^\delta)$ is the subspace of $H^1(Y_K^\delta)$ consisting of d -periodic functions with zero mean value. $f_K := 1/|K| \int_K$ denotes the arithmetic average.

The purpose of this paper is to discuss a novel approach of determining the effective values A^δ (for a given sampling discretization) by means of an optimization process. It will be based on an error identity given by the solution of a dual problem. For the sake of simplicity, we will neglect *finescale discretization* errors that emerge by numerically approximating (2.5), or (2.7), and will only introduce a macroscale discretization.

Let $\mathbb{T}_H(\Omega)$ be a coarse grid for numerically approximating the variational equation (2.3).

DEFINITION 2.2 (Fully discretized problem). *Let \mathbb{T}_H be a mesh covering $\overline{\Omega}$, and let $V_H(\Omega) \subset H_0^1(\Omega)$ be a corresponding finite-element ansatz space. The fully discrete problem reads: Find $U \in V_H(\Omega)$ s. t.*

$$(2.8) \quad (A^\delta \nabla U, \nabla \varphi^H) = (f, \varphi^H) \quad \forall \varphi^H \in V_H(\Omega).$$

REMARK 2.3. *The problems (2.1), (2.3), and (2.8) are well-posed. Further, specific a priori assumptions on A^ε and corresponding concrete choices of upscaling (such as (2.5), and (2.7)) lead to different a priori error estimates. We refer to [16, 17], for a detailed discussion.*

2.1. Duality-based error identity. Suppose that a *quantity of interest* is given by the value $\langle j, u^\varepsilon \rangle$, where $j \in H^{-1}(\Omega)$ is a linear and continuous functional and $\langle \cdot, \cdot \rangle$ denotes the duality pairing. Define a *dual problem* to find $z^\varepsilon \in H_0^1(\Omega)$ s. t.

$$(2.9) \quad (A^\varepsilon \nabla \varphi, \nabla z^\varepsilon) = \langle j, \varphi \rangle \quad \forall \varphi \in H_0^1(\Omega).$$

The dual problem is well-posed and its solution immediately gives rise to an *error identity*.

LEMMA 2.4 (Error identity [16, 17]). *Let u^ε be the solution of (2.1), U be the solution of (2.8), and z^ε be the solution of (2.9). Then,*

$$(2.10) \quad \langle j, u^\varepsilon \rangle - \langle j, U \rangle = \underbrace{(f, z^\delta) - (A^\delta \nabla U, \nabla z^\delta)}_{=: \theta^H} + \underbrace{(A^\delta \nabla u^\delta, \nabla z^\varepsilon) - (A^\varepsilon \nabla u^\delta, \nabla z^\varepsilon)}_{=: \theta^\delta},$$

with the following two error estimators: θ^H representing a residual on the macroscale, and θ^δ estimating the model error. Here, $z^\delta \in H_0^1(\Omega)$ is the solution of a corresponding effective dual problem [17],

$$(2.11) \quad (A^\delta \nabla \varphi, \nabla z^\delta) = \langle j, \varphi \rangle \quad \forall \varphi \in H_0^1(\Omega).$$

The model error θ^δ is splitted into a sum of local model-error indicators:

$$(2.12) \quad \theta^\delta = \sum_{K \in \mathbb{T}_\delta(\Omega)} \eta_K^\delta, \quad \eta_K^\delta := (\{A^\varepsilon - A^\delta\} \nabla u^\delta, \nabla z^\varepsilon)_K.$$

2.2. A localization strategy for the dual problem. A fundamental difficulty arises from the fact that computing the solution of the dual problem is (in case of the elliptic model problem) of the same complexity as the primal problem itself. A global fine-scale approximation of z^ε has to be considered infeasible. Thus, a strategy to approximate the dual problem with low computational overhead is needed.

We proposed [16, 17] a strategy that combines the usage of a global, effective approximation of z^ε (such as z^δ) with a local enhancement. The enhancement is given by localized reconstruction problems in spirit of a *variational multiscale* ansatz.

DEFINITION 2.5 (Local enhancement). *Let z^δ be the solution of (2.11),*

$$(2.13) \quad (A^\delta \nabla \varphi, \nabla z^\delta) = \langle j, \varphi \rangle \quad \forall \varphi \in H_0^1(\Omega),$$

and let $\{\omega_K : K \in \mathbb{T}_\delta(\Omega)\}$ be a set of reconstruction patches fulfilling $\omega_K \supset K$. Define a patch-wise reconstruction $z_K^\delta \in H_0^1(\omega_K)$ by

$$(2.14) \quad (A^\varepsilon \nabla \varphi, \nabla (z^\delta + z_K^\delta)) = \langle j, \varphi \rangle \quad \forall \varphi \in H_0^1(\omega_K).$$

With the choice $\omega(K) = K$, the locally reconstructed dual solution leads to a conforming ansatz $z^\delta + \sum_{K \in \mathbb{T}_\delta} z_K^\delta \in H^1(\Omega)$. In this case the above local enhancement strategy can be regarded as a variant of the VMM formulation that only has a reconstruction coupling from coarse- to finescale (and omits the opposite compression coupling).

In contrast to residual-type estimators that can be evaluated in a simple post-processing step, the practical evaluation of the error estimators require the approximation of an additional, intermediate dual solution and effective coefficients; for details we refer to [16, 17].

3. Model-optimization framework. In the previous section an error identity and local error estimates were introduced for the model error, as well as, the macroscale discretization error. The treatment of discretization errors by adaptive mesh refinement with the help of local error indicators is well established [4, 5]. The question arises what to do in case of the model error: Based on the concept of the effective model

$$(3.1) \quad \bar{A}^\delta : \mathbb{T}_\delta(\Omega) \rightarrow \mathbb{R}^{d \times d},$$

two fundamentally different approaches for model adaptivity are possible. The first is based on the refinement of the sampling mesh $\mathbb{T}_\delta(\Omega)$ and associated sampling regions $\{Y_K^\delta : K \in \mathbb{T}_\delta(\Omega)\}$ while keeping the same reconstruction process for all sampling regions [17]. This is comparable to a classical discretization adaptation. The second strategy consists of switching the effective model used for the reconstruction process [6, 19–21]. This is done by locally selecting a more expensive but also more precise sampling strategy from an a priori chosen list of effective models. Typically, the same fixed sampling discretization is used throughout the process.

In this section a novel approach for model adaptivity is introduced that expresses the adaptation process as a *minimization problem* of the error estimator θ^δ : Given the *error identity* (2.10),

$$(3.2) \quad \langle j, u^\varepsilon \rangle - \langle j, U \rangle = \theta^H + \theta^\delta, \quad \theta^\delta = ((A^\delta - A^\varepsilon) \nabla u^\delta, \nabla z^\varepsilon),$$

model adaptivity is interpreted as solving an *optimization problem*

$$(3.3) \quad \arg \inf_{A^\delta} \sum_{K \in \mathbb{T}_\delta(\Omega)} \left[|((A^\delta - A^\varepsilon) \nabla u^\delta, \nabla z^\varepsilon)_K|^2 + \text{regularization} \right].$$

This approach can be used as a *model-optimization framework* to locally select optimal coefficients from a set of available models, as well as in situations where a strategy to derive an effective model is not known and, thus, an efficient post-processing strategy is needed to construct one. The latter approach has the advantage that no a priori knowledge about effective models and reconstruction principles has to be available. The optimization problem itself is used to select the optimal model.

3.1. An optimization approach. The *quality* of an effective model A^δ with respect to a *quantity of interest* $\langle j, u^\varepsilon \rangle$ can be measured with the help of the error identity (2.10):

$$(3.4) \quad \langle j, u^\varepsilon \rangle - \langle j, u^\delta \rangle = ((A^\delta - A^\varepsilon) \nabla u^\delta(\bar{A}^\delta), \nabla z^\varepsilon)_{L^2(\Omega)^d}.$$

Given a fixed, a priori chosen sampling discretization $\mathbb{T}_\delta(\Omega)$, define a set of *admissible coefficients* consisting of symmetric and elliptic coefficient tensors (as defined in (2.2),

$$(3.5) \quad \mathcal{A}^\delta := \{\bar{A}^\delta : \mathbb{T}_\delta(\Omega) \rightarrow \mathbb{R}^{d \times d} : \bar{A}^\delta \text{ fulfills (2.2)}\}.$$

DEFINITION 3.1 (Model-optimization problem). *Let $\bar{A}^{\delta,0}$ be an initial effective model and let $\{\alpha_K\}_{K \in \mathbb{T}_\delta(\Omega)}$, $\alpha_K \in \mathbb{R}^+$, be a set of (local) regularization parameters. Then, an optimal model $\bar{A}^{\delta,opt}$ is defined to be a solution of*

$$(3.6) \quad \arg \inf_{\bar{A}^\delta \in \mathcal{A}^\delta} \sum_{K \in \mathbb{T}_\delta(\Omega)} \left\{ |((\bar{A}^\delta - A^\varepsilon) \nabla u^\delta(\bar{A}^\delta), \nabla z^\varepsilon)_K|^2 + \alpha_K \|\bar{A}_K^\delta - \bar{A}_K^{\delta,0}\|_{\mathbb{R}^{d \times d}}^2 \right\},$$

subject to the side condition

$$(3.7) \quad (\bar{A}^\delta \nabla u^\delta(\bar{A}^\delta), \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega).$$

The regularization parameters α_K are best fixed to a uniform value $\alpha_K = \alpha_0$ on all sampling regions. Here, α_0 is chosen to be roughly 0.01 – 1 times the typical size of $|\hat{\theta}^\delta|^2 / |\bar{A}_K^\delta|^2$.

REMARK 3.2. *Given the fact that ellipticity (2.2) is impractical to enforce, because the correct lower-bound α is usually not known, the ellipticity constraint present in \mathcal{A}^δ is dropped in the concrete numerical computations. The regularization together with a factor α_K appropriately chosen is enough to ensure sensible coefficients \bar{A}^δ .*

PROPOSITION 3.3. *The optimization problem admits a (not necessarily unique) minimum.*

Proof. The functional dependency $u^\delta(\bar{A}^\delta)$ described by (3.7) with respect to $\bar{A}^\delta \in \mathcal{A}^\delta$ is well-posed—i. e., (3.7) is always uniquely solvable—and continuous. Further,

$$(3.8) \quad \|\nabla u^\delta(\bar{A}^\delta)\| \leq \frac{1}{\alpha} \|f\|,$$

by definition of \mathcal{A}^δ . Hence, the function

$$(3.9) \quad \mathcal{F}(\bar{A}^\delta) := \sum_{K \in \mathbb{T}_\delta(\Omega)} \left\{ |((\bar{A}^\delta - A^\varepsilon) \nabla u^\delta(\bar{A}^\delta), \nabla z^\varepsilon)_K|^2 + \alpha_K \|\bar{A}_K^\delta - \bar{A}_K^{\delta,0}\|_{\mathbb{R}^{d \times d}}^2 \right\}$$

is well-defined, continuous, and coercive, i. e., it holds true that

$$(3.10) \quad \mathcal{F}(\bar{A}^\delta) \rightarrow \infty \quad \text{for} \quad \|\bar{A}^\delta\| \rightarrow \infty.$$

The optimization problem thus possesses a minimizer. \square

REMARK 3.4. *The functional dependency $u^\delta(\bar{A}^\delta)$ given by the side-condition (3.7) is highly nonlinear. In fact, $\|\nabla u^\delta\|_{L^2(K)} \rightarrow 0$ has to be expected for the limit $\|\bar{A}_K^\delta\| \rightarrow \infty$. Consequently, the term $|((\bar{A}^\delta - A^\varepsilon) \nabla u^\delta(\bar{A}^\delta), \nabla z^\varepsilon)_K|^2$ is generally not convex. The optimization problem is therefore not uniquely solvable in general.*

In preparation for the numerical treatment of the optimization problem (3.6), we formulate the following regularity result for the cost functional \mathcal{F} given in (3.9).

PROPOSITION 3.5. *The functional dependency $\mathcal{F}(\bar{A}^\delta)$ is Gâteaux-differentiable and its derivative $D\mathcal{F}(\bar{A}^\delta)[\delta\bar{A}^\delta]$ in direction $\delta\bar{A}^\delta$ is given by*

$$(3.11) \quad D\mathcal{F}(\bar{A}^\delta)[\delta\bar{A}^\delta] = \sum_{K \in \mathbb{T}_\delta(\Omega)} \left\{ 2\eta_K^\delta (\delta\bar{A}_K^\delta \nabla u^\delta(\bar{A}^\delta), \nabla z^\varepsilon)_K \right. \\ \left. + 2\eta_K^\delta ((\bar{A}^\delta - A^\varepsilon) \nabla D u^\delta(\bar{A}^\delta)[\delta\bar{A}^\delta], \nabla z^\varepsilon)_K \right. \\ \left. + 2\alpha_K (\bar{A}_K^\delta - \bar{A}_K^{\delta,0}) : \delta\bar{A}_K^\delta \right\},$$

with the solution $Du^\delta(\bar{A}^\delta)[\delta\bar{A}^\delta]$ of the equation

$$(3.12) \quad (\bar{A}^\delta \nabla D u^\delta(\bar{A}^\delta)[\delta\bar{A}^\delta], \nabla \varphi) + (\delta\bar{A}^\delta \nabla u^\delta(\bar{A}^\delta), \nabla \varphi) = 0 \quad \forall \varphi \in H^1(\Omega).$$

Proof. The crucial part is to assert that the side condition (3.7) interpreted as a functional dependency $u^\delta(\bar{A}^\delta)$ is Gâteaux-differentiable and its derivative is given by (3.12). The rest of the statement then follows in a straightforward manner. Due to the fact that \mathcal{A}^δ is finite dimensional it suffices to show that the limit

$$(3.13) \quad \lim_{s \searrow 0} D_s u^\delta, \quad D_s u^\delta := \frac{1}{s} (u^\delta(\bar{A}^\delta + s\delta\bar{A}^\delta) - u^\delta(\bar{A}^\delta))$$

is well-defined for arbitrary $\delta\bar{A}^\delta$. For this, we note that the difference $D_s u^\delta(\bar{A}^\delta)$ is, for s sufficiently small, given by

$$(3.14) \quad ((\bar{A}^\delta + s\delta\bar{A}^\delta) \nabla (u^\delta(\bar{A}^\delta) + sD_s u^\delta), \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H^1(\Omega).$$

Equivalently,

$$(3.15) \quad (\bar{A}^\delta \nabla D_s u^\delta, \nabla \varphi) + s (\delta\bar{A}^\delta \nabla D_s u^\delta, \nabla \varphi) + (\delta\bar{A}^\delta u^\delta(\bar{A}^\delta), \nabla \varphi) = 0.$$

By continuity, it follows that the limit of (3.15) for $s \rightarrow 0$ is well-defined and indeed given by (3.12). \square

3.2. An efficient post-processing strategy. The optimization problem (3.6) can be used as an efficient post-processing strategy that does not require—with the exception of an initial model—any additional a priori knowledge of effective models. Fix a macroscale and a sampling discretization $\mathbb{T}_H(\Omega)$ and $\mathbb{T}_\delta(\Omega)$, as well as an initial effective coefficients $\bar{A}^{\delta,0}$. This results in the following general optimization strategy formulated for the case of a reduced, locally enhanced approximation of the dual solution:

DEFINITION 3.6 (Reduced, locally enhanced model-optimization problem).

Let $\mathbb{T}_\delta(\Omega)$ be a fixed sampling mesh and $\mathbb{T}_H(\Omega)$ a fixed macroscale discretization. Fix a microscale discretization $\{\mathbb{T}_h(K) : K \in \mathbb{T}_\delta(\Omega)\}$ as well and let $\bar{A}^{\delta,0} : \mathbb{T}_\delta(\Omega) \rightarrow \mathbb{R}^{d \times d}$ be an initial effective model. The reduced, locally enhanced model-optimization problem reads: Find a solution $\bar{A}^{\delta,opt} \in \mathcal{A}^\delta$ of

$$(3.16) \quad \arg \inf_{\bar{A}^\delta \in \mathcal{A}^\delta} \sum_{K \in \mathbb{T}_\delta(\Omega)} \left\{ |((\bar{A}^\delta - A^\varepsilon) \nabla U(\bar{A}^\delta), \nabla(\tilde{Z} + \tilde{Z}_K)(\bar{A}^\delta))_K|^2 \right. \\ \left. + \alpha_K \|\bar{A}_K^\delta - \bar{A}_K^{\delta,0}\|_{\mathbb{R}^{d \times d}}^2 \right\},$$

with $U, \tilde{Z} \in V^H(\Omega)$, and $\tilde{Z}_K \in V^h(K)$ subject to the side conditions:

$$(3.17) \quad (\bar{A}^\delta \nabla U(\bar{A}^\delta), \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in V^H(\Omega),$$

$$(3.18) \quad (\bar{A}^\delta \nabla \varphi, \nabla \tilde{Z}(\bar{A}^\delta)) = \langle j, \varphi \rangle \quad \forall \varphi \in V^H(\Omega),$$

$$(3.19) \quad (A^\varepsilon \nabla \varphi, \nabla \tilde{Z} + \nabla \tilde{Z}_K)_K = \langle j, \varphi \rangle \quad \forall \varphi \in V^h(K).$$

Analogously to Proposition 3.5 we formulate the following result:

PROPOSITION 3.7. *Let $\tilde{\mathcal{F}}$ be the modified cost functional of (3.16). Then, in full analogy of the result for \mathcal{F} in Proposition 3.5, the functional dependency of $\tilde{\mathcal{F}}(\bar{A}^\delta)$ is also Gâteaux-differentiable and it holds true that*

$$(3.20) \quad D\tilde{\mathcal{F}}(\bar{A}^\delta)[\delta \bar{A}^\delta] = D\mathcal{F}(\bar{A}^\delta, U, \tilde{Z})[\delta \bar{A}^\delta] + \sum_{K \in \mathbb{T}_\delta(\Omega)} 2\eta_K^\delta ((\bar{A}^\delta - A^\varepsilon) \nabla U, \nabla (D\tilde{Z} + D\tilde{Z}_K)(\bar{A}^\delta)[\delta \bar{A}^\delta]),$$

with $D\tilde{Z} \in V^H(K)$ being defined as the solution of

$$(3.21) \quad (\bar{A}^\delta \nabla \varphi, \nabla D\tilde{Z}(\bar{A}^\delta)[\delta \bar{A}^\delta]) + (\delta \bar{A}^\delta \nabla \varphi, \nabla \tilde{Z}(\bar{A}^\delta)) = 0 \quad \forall \varphi \in V^H(\Omega),$$

and $D\tilde{Z}_K \in V^h(K)$ solving

$$(3.22) \quad (A^\varepsilon \nabla \varphi, \nabla D\tilde{Z}_K(\bar{A}^\delta)[\delta \bar{A}^\delta])_K + (A^\varepsilon \nabla \varphi, \nabla \delta \tilde{Z}(\bar{A}^\delta)[\delta \bar{A}^\delta])_K = 0 \quad \forall \varphi \in V^h(K).$$

Proof. The first part of the statement is already proved in Proposition 3.5. The additional terms arise from the derivatives of Equations (3.18) and (3.19). \square

4. Implementational aspects. The optimization problem (3.6) and its modified variant (3.16) contain strongly nonlinear side conditions, where computing the Gâteaux-derivative for a given direction $\delta \bar{A}^\delta$ alone already involves solving the variational equation (3.12), and, depending on the reconstruction approach, also (3.21) and (3.22). Consequently, a straightforward application of the *Newton method* to solve the optimization problem has to be avoided.

4.1. Gauß-Newton Method. In order to avoid computing the second order derivatives $d^2\mathcal{F}(\bar{A}^{\delta,i})$ a *modified Gauß-Newton method* [18] is used. For this, we reformulate the optimization problem slightly. Introduce a multi-index $(K, i, j) \in \mathbb{T}_\delta \times \mathbb{R}^{d \times d}$ and define the vector-valued function

$$(4.1) \quad \mathcal{G} := \{(\eta_K)_K, (g_{Kij})_{Kij}\}, \quad \text{with}$$

$$(4.2) \quad \eta_K := ((\bar{A}^\delta - A^\varepsilon) \nabla U(\bar{A}^\delta), \nabla (\tilde{Z} + \tilde{Z}_K))_K, \quad g_{Kij} := \sqrt{\alpha_K} (\bar{A}_{K,ij}^\delta - \bar{A}_{K,ij}^{\delta,0}).$$

LEMMA 4.1. *The modified optimization problem (3.16) can equivalently be expressed as the minimization of the squared Euclidian norm $|\cdot|$ of \mathcal{G} :*

$$(4.3) \quad \arg \inf_{\bar{A}^\delta \in \mathcal{A}^\delta} |\mathcal{G}|^2 = \arg \inf_{\bar{A}^\delta \in \mathcal{A}^\delta} \sum_{K \in \mathbb{T}_\delta(\Omega)} \left\{ \eta_K^2 + \sum_{ij} g_{Kij}^2 \right\}.$$

For a given index (K, i, j) let $\delta \bar{A}^\delta(Kij) : \mathbb{T}_\delta \rightarrow \mathbb{R}^{d \times d}$ be defined as the value

$$(4.4) \quad (\delta \bar{A}_Q^\delta)_{mn} := \delta_{QK} \delta_{mi} \delta_{ni},$$

for a cell $Q \in \mathbb{T}_\delta(\Omega)$, where δ_{QK} is the *Kronecker delta*. Define the short notation

$$(4.5) \quad D_{Kij} \eta_Q := D\eta_Q[\delta \bar{A}^\delta(Kij)],$$

$$(4.6) \quad D_{Kij} g_{Qmn} := Dg_{Qmn}(\bar{A}^\delta)[\delta \bar{A}^\delta(Kij)].$$

LEMMA 4.2. *By virtue of Propositions 3.5 and 3.7 it holds that*

$$(4.7) \quad \begin{aligned} D_{Kij} \eta_Q &= \delta_{QK} \int_Q \nabla_j U \nabla_i (\tilde{Z} + \tilde{Z}_Q) dx \\ &\quad + \int_Q (\bar{A}^\delta - A^\varepsilon) \nabla D_{Kij} U \cdot \nabla (\tilde{Z} + \tilde{Z}_Q) dx \\ &\quad + \int_Q (\bar{A}^\delta - A^\varepsilon) \nabla U \cdot \nabla D_{Kij} (\tilde{Z} + \tilde{Z}_Q) dx, \end{aligned}$$

as well as

$$(4.8) \quad D_{Kij} g_{Qmn} = \delta_{QK} \delta_{mi} \delta_{ni} \sqrt{\alpha_Q}.$$

With these prerequisites at hand, a modified Gauß-Newton iteration following a discussion by Levenberg and Marquardt [18] is defined:

DEFINITION 4.3 (Gauß-Newton iteration). *Let \mathcal{J} be the Jacobian matrix of \mathcal{G} ,*

$$(4.9) \quad \mathcal{J} = \left\{ (D_{Kij} \eta_Q)_Q^{Kij}, (D_{Kij} g_{Qmn})_Q^{Kij} \right\}.$$

Given a penalty $\lambda \geq 0$ and starting from an initial effective model $\bar{A}^{\delta,0}$ the modified Gauß-Newton iteration reads

$$(4.10) \quad \begin{cases} \bar{A}^{\delta,n+1} \leftarrow \bar{A}^{\delta,n} + \delta \bar{A}^{\delta,n}, \\ (\mathcal{J} \mathcal{J}^T (\bar{A}^{\delta,n}) + \lambda Id) \delta \bar{A}^{\delta,n} = -\mathcal{J} \mathcal{G}^T (\bar{A}^{\delta,n}). \end{cases}$$

The penalization term λId acts as a damping term in the Gauß-Newton method to stabilize the iteration and to reduce the influence of approximation errors of the Jacobian \mathcal{J} . Depending on the situation, it will be chosen between 0 – 1 times the mean value of the diagonal elements of $\mathcal{J} \mathcal{J}^T$.

4.2. Reduction of computational complexity. The computationally expensive part of computing the Jacobi matrix \mathcal{J} are the non-local responses $D_{Kij} U$, $D_{Kij} \tilde{Z}$, and $D_{Kij} \tilde{Z}_Q$ that have to be computed for each choice (K, i, j) individually according to (3.12), (3.21), and (3.22). Another aspect that has to be kept in mind is the fact that $\mathcal{J} \mathcal{J}^T$ is actually a dense matrix of size $N \times N$ with $N = |\mathbb{T}_\delta(\Omega)| (1+d^2)$. Storing such a matrix, even for moderate sizes of the sampling mesh $\mathbb{T}_\delta(\Omega)$, is computationally infeasible. Thus, a reduction strategy to efficiently approximate \mathcal{J} is necessary.

The microscale response $D_{Kij} U$ is given by (cf. Equation 3.12):

$$(4.11) \quad (\bar{A}^\delta \nabla D_{Kij} U, \nabla \varphi) = - \int_K \nabla_j U \nabla_i \varphi dx \quad \forall \varphi \in V^H(\Omega).$$

The right hand side of this equation is highly localized. Consequently, the contribution of

$$(4.12) \quad \int_Q (\bar{A}^\delta - A^\varepsilon) \nabla D_{Kij} U \cdot \nabla (\tilde{Z} + \tilde{Z}_Q) dx$$

rapidly decreases the farther Q is away from K —and can be neglected at some point. A sensible compromise is, for example, to compute the above contribution only for the case $K = Q$, or alternatively, as a more precise strategy, only if Q belongs to a small patch around K , e.g., if $\bar{K} \cap \bar{Q} \neq \emptyset$. All of these choices result in a block diagonal matrix $\tilde{\mathcal{J}}$ whose *band size* is independent of $|\mathbb{T}_\delta(\Omega)|$.

In contrast the microscale response $D\tilde{Z}$, $D\tilde{Z}_Q$ will just be neglected entirely:

$$(4.13) \quad \int_Q (\bar{A}^\delta - A^\varepsilon) \nabla U \cdot \nabla D_{Kij} (\tilde{Z} + \tilde{Z}_Q) dx \approx 0.$$

The reasoning behind this choice is the fact that in case of a fully resolved dual solution z^ε , such finescale response does not exist at all. Further, the optimization problem (3.16) is designed to be an approximation of (3.6). Hence a derivative approximation (probably) closer to the original problem is actually desirable. In summary, the following approximation strategies of the derivative $D_{Kij}\eta_Q$ will be considered:

DEFINITION 4.4 (Approximative Jacobian). *Define a patch $\omega(K) := \{Q \in \mathbb{T}_\delta(\Omega) : \bar{K} \cap \bar{Q} \neq \emptyset\}$ and let $I_{Q\omega(K)}$ be the indicator function that is equal to 1 for $Q \in \omega(K)$ and 0 otherwise. The derivative $D_{Kij}\eta_Q$ is approximated by*

$$(4.14) \quad D_{Kij}\eta_Q \approx \delta_{QK} \int_Q \nabla_j U \nabla_i (\tilde{Z} + \tilde{Z}_Q) dx \\ + I_{Q\omega(K)} \int_Q (\bar{A}^\delta - A^\varepsilon) \nabla D_{Kij} U \cdot \nabla (\tilde{Z} + \tilde{Z}_Q) dx.$$

One last obstacle for the patch-centered reconstruction (4.14) remains. Namely, that the response $D_{Kij}U$ is needed in combination with the microscale reconstruction \tilde{Z}_Q for different K and Q . In an efficient algorithm, fine-scale reconstructions of such kind cannot be stored for further use. They have to be kept local to the computation on the current sampling region Q . One way to mitigate this problem is to not use a finescale reconstruction Z_Q defined on Q , but to use a slightly more expensive $\tilde{Z}_{\omega(K)}$ defined on the patch $\omega(K)$ around K with patch-depth 1. This allows for an efficient assembly as described in Algorithm 1. Finally, a model-optimization algorithm can be defined; see Algorithm 2.

REMARK 4.5. *Due to the fact that \mathcal{J} is always approximated with a substantially reduced variant, the value $\|\mathcal{J}\|$ does not provide a good stopping criterion with $\|\mathcal{J}\| \ll 1$. Instead, it is better to use the approximative estimator value $|\tilde{\theta}^\delta|$ directly. For example, stop if $|\tilde{\theta}^\delta|$ is reduced to 1% of its initial value.*

5. Numerical tests. A series of short numerical tests is conducted in order to examine specific behavior and aspects of the model-optimization approach that was proposed in the previous sections. The computations are done with the finite-element toolkit deal.II [3].

In particular, the dependence of the optimization result on the initial value $\bar{A}^{\delta,0}$, on the size of the sampling discretization $\mathbb{T}_\delta(\Omega)$, and on the strength of the regularization parameters α_K is examined for a global functional, as well as a local variant

Algorithm 1: Assembly of $\{\eta_K\}$ and \mathcal{J}

-
- Set up $\mathbb{T}_H(\Omega)$ and assemble matrix A : $A_{\nu\mu} = (\bar{A}^{\delta,i} \nabla \varphi_\mu, \nabla \varphi_\nu)$
 - Compute matrix decomposition of A : $LU = A$
 - for** $K \in \mathbb{T}_\delta(\Omega)$ **do**
 - Assemble $\omega(K)$ and compute $\tilde{Z}_K \in V^h(\omega(K))$
 - Compute η_K^δ with (2.12)
 - for** $i = 1, \dots, d$ **do**
 - for** $j = 1, \dots, d$ **do**
 - Compute response $D_{Kij}U$ with above decomposition
 - for** $Q \in \omega(K)$ **do**
 - Compute contribution $D_{Kij}\eta_Q$ for \mathcal{J} according to (4.14)
-

Algorithm 2: Model-optimization algorithm

-
- Compute initial model $\bar{A}^{\delta,0}$
 - Solve primal and dual problem for $U(\bar{A}^{\delta,0}), \tilde{Z}(\bar{A}^{\delta,0})$ with the help of (2.8)
 - while** *stopping criterion not reached* **do**
 - Compute the error estimator and local indicators $\{\eta_K\}$
$$\tilde{\theta}^\delta = \sum_{K \in \mathbb{T}_\delta(\Omega)} \eta_K^\delta,$$

as well as, the Jacobian \mathcal{J} with Algorithm 1

 - Solve $(\mathcal{J} \mathcal{J}^T(\bar{A}^{\delta,n}) + \lambda \text{Id}) \delta \bar{A}^{\delta,n} = -\mathcal{J} \mathcal{G}^T(\bar{A}^{\delta,n})$.
 - Update model: $\bar{A}^{\delta,n+1} \leftarrow \bar{A}^{\delta,n} + \delta \bar{A}^{\delta,n}$
 - Compute $U(\bar{A}^{\delta,n+1}), \tilde{Z}(\bar{A}^{\delta,n+1})$ again with updated model $\bar{A}^{\delta,n+1}$, (2.8)
-

(Subsection 5.1). This is done with a choice of random coefficients for both, the fully resolved dual solution z^ε , as well as the reduced, locally enhanced variant $z^\delta + \sum z_K^\delta$. Finally, Subsection 5.2 concludes with an advection-diffusion example with dominant transport.

5.1. Parameter study for random coefficients. The purpose of the first numerical test is to examine the stability of the optimization approach for a variety of differently chosen discretization and optimization parameters. In particular, the feasibility of using the reduced, locally enhanced approximation approach within the optimization framework shall be assessed as this property is essential for the optimization approach to be computationally feasible and thus comparable to VMM or HMM approaches.

Consider a computational domain $\Omega = (0, 1)^2$ with a log-normally distributed, random microstructure. In detail, we choose A^ε to be

$$(5.1) \quad A^\varepsilon(x) := I_d \times \gamma \times \exp(10 \times g(x) / 255) I_d,$$

where $g(x)$ is an 8 bit grayscale picture (with integral values between 0 and 255)

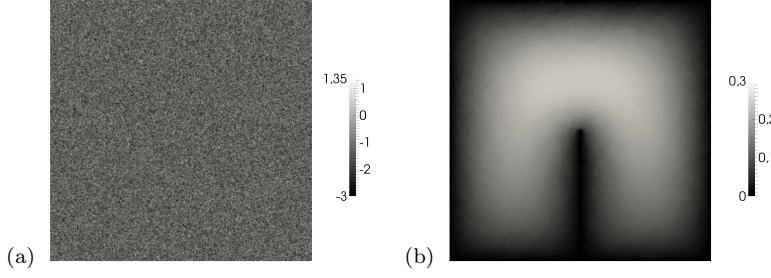


Figure 2: (a) Log-normally distributed permeability with Gaussian correlation shown in log-scale. (b) The corresponding reference solution.

with 1024×1024 pixels resolution (cf. Fig. 2). The grayscale picture is generated using the `QuantIm` library [22]. It is a (discrete) Gaussian random field with an additional Gaussian correlation with a correlation length chosen to be $r = 0.0025$.

Further, define a global and a local functional as follows:

$$(5.2) \quad \langle j_1, \varphi \rangle = \int_{\Omega} \varphi \, dx, \quad \langle j_2, \varphi \rangle = \varphi(x_0).$$

For a fixed choice of $65.5K$ macrocells and a microscale resolution of $h = 2^{-12}$, a parameter study is conducted with sampling discretizations $\delta = 2^{-3}$ and $\delta = 2^{-4}$, a choice of mild penalty with $\lambda = 0.1m$ and regularization $\alpha_K = 0.001$ and strong penalty $\lambda = 1.0m$ and regularization $\alpha_K = 0.01$, where m is the absolute mean value of the diagonal entries of the matrix $\mathcal{J}^T \mathcal{J}$, see (4.10). The optimization algorithm is run for the optimization strategy with precise approximative Jacobian (4.14) for both types of reconstruction approaches for the dual solution: fully resolved z^ε and the reduced, local enhanced variant $z^\delta + \sum z_K^\delta$. With reference values of $\langle j_1, u_{\text{ref}}^\varepsilon \rangle \approx 0.14641$ and $\langle j_2, u_{\text{ref}}^\varepsilon \rangle \approx 0.189403$ the initial model errors are in the range of around 1% for the geometric average.

For each choice of parameters, Table 1 shows the final error after a fixed number of 15 optimization cycles for periodic and random coefficients. The first observation that can be made is that in all cases the model-optimization approach is able to consistently reduce well below 1%. More importantly, the reduced, locally enhanced variant $z^\delta + \sum z_K^\delta$ with increased patch size (and thus reduced impact of the artificial Dirichlet boundary conditions of the reconstruction problems) leads to comparable results very similar to the results for the full variant z^ε .

5.2. An advection-diffusion example with dominant transport. As second test case consider an *advection-diffusion* problem

$$(5.3) \quad \gamma (\nabla u^\varepsilon, \nabla \varphi) + (\mathbf{b}^\varepsilon \cdot \nabla u^\varepsilon, \varphi) = (f, \varphi) \quad \forall \varphi \in V$$

driven by a divergence-free vector field $\mathbf{b}^\varepsilon \in H^{1,\infty}(\Omega)^d$, i.e. $\nabla \cdot \mathbf{b}^\varepsilon = 0$ a.e. on Ω and $\mathbf{b}^\varepsilon \equiv 0$ on $\partial\Omega$, together with a positive scaling factor $\gamma \in \mathbb{R}^+$. This time, the multiscale character is given by \mathbf{b}^ε that shall consist of small (but strong) eddies. We again use the `QuantIm` library [22] to construct a random, divergence-free vector field $\mathbf{b}^\varepsilon(\mathbf{x})$; see [16]. For a given sampling discretization $\mathbb{T}_\delta(\Omega)$, we define an averaged

Table 1: Parameter study for a random permeability and the global functional j_1 , as well as the local functional j_2 . For each choice the absolute and relative error after cycle 15 of the optimization algorithm is shown.

(a) Full model-optimization (4.14), geometric average $\bar{A}^{\delta,0}$, global functional j_1					
	cycle	z^ε		$z^\delta + \sum z_K^\delta$	
		$\delta = 2^{-3}$	$\delta = 2^{-4}$	$\delta = 2^{-3}$	$\delta = 2^{-4}$
	1	1.8e-3 (1.3 %)	1.3e-3 (0.9 %)	1.8e-3 (1.3 %)	1.3e-3 (0.9 %)
$\alpha_K = 10^{-2}$	15	7.5e-4 (0.5 %)	4.2e-4 (0.3 %)	6.7e-4 (0.5 %)	3.7e-4 (0.3 %)
$\alpha_K = 10^{-3}$	15	8.0e-4 (0.6 %)	7.9e-4 (0.5 %)	7.1e-4 (0.5 %)	7.2e-4 (0.5 %)

(b) Full model-optimization (4.14), geometric average $\bar{A}^{\delta,0}$, local functional j_2					
	cycle	z^ε		$z^\delta + \sum z_K^\delta$	
		$\delta = 2^{-3}$	$\delta = 2^{-4}$	$\delta = 2^{-3}$	$\delta = 2^{-4}$
	1	2.1e-3 (1.1 %)	2.2e-3 (1.2 %)	2.1e-3 (1.1 %)	2.2e-3 (1.2 %)
$\alpha_K = 10^{-2}$	15	6.0e-4 (0.3 %)	6.2e-4 (0.3 %)	8.7e-4 (0.5 %)	9.5e-4 (0.5 %)
$\alpha_K = 10^{-3}$	15	6.9e-4 (0.4 %)	7.2e-4 (0.4 %)	9.5e-4 (0.5 %)	1.0e-3 (0.5 %)

transport coefficient

$$(5.4) \quad \mathbf{b}^\delta : \mathbb{T}_\delta(\Omega) \rightarrow \mathbb{R}^d, \quad \mathbf{b}_K^\delta := \oint_K \mathbf{b}^\varepsilon dx \quad \text{for } K \in \mathbb{T}_\delta(\Omega).$$

The random advection field influences the macroscopic diffusion in two ways. Firstly, an averaged macroscopic transport occurs (as described by \mathbf{b}^δ). Secondly, and more importantly, the microscopic eddies lead to influence the macroscopic behavior by means of an additional *effective diffusivity*. Consequently, let the task be to find effective (diffusion) coefficients $\bar{A}^\delta : \mathbb{T}_\delta(\Omega) \rightarrow \mathbb{R}^{d \times d}$ such that the solution u^δ of the *effective advection-diffusion problem*

$$(5.5) \quad (\bar{A}^\delta \nabla u^\delta, \nabla \varphi) + (\mathbf{b}^\delta \cdot \nabla u^\delta, \varphi) = (f, \varphi) \quad \forall \varphi \in V,$$

is a good approximation of u^ε in some quantity of interest.

The only significant change in the model-adaptation framework for the above advection-diffusion problem is the occurrence of additional terms $(\mathbf{b}^\varepsilon \cdot \nabla u^\varepsilon, z^\varepsilon)$ in the error identity (2.10) that now splits into

$$(5.6) \quad \langle j, u^\varepsilon \rangle - \langle j, U \rangle = \underbrace{(f, z^\delta) - (A^\delta \nabla U, \nabla z^\delta) - (\mathbf{b}^\delta \cdot \nabla U, z^\delta)}_{=: \theta^H} + \underbrace{(A^\delta \nabla u^\delta, \nabla z^\varepsilon) - \gamma (\nabla u^\delta, \nabla z^\varepsilon) - ((\mathbf{b}^\varepsilon - \mathbf{b}^\delta) \cdot \nabla u^\delta, z^\varepsilon)}_{=: \theta^\delta}$$

This leads to a local model-error indicator

$$(5.7) \quad \eta_K^\delta := (\{\gamma \text{Id} - A^\delta\} \nabla u^\delta, \nabla z^\varepsilon)_K - ((\mathbf{b}^\varepsilon - \mathbf{b}^\delta) \cdot \nabla u^\delta, z^\varepsilon)_K.$$

With the above assumptions on \mathbf{b}^ε the corresponding dual problem reads

$$(5.8) \quad \gamma (\nabla \varphi, \nabla z^\varepsilon) - (\mathbf{b}^\varepsilon \cdot \nabla z^\varepsilon, \varphi) = \langle j, \varphi \rangle \quad \forall \varphi \in V.$$

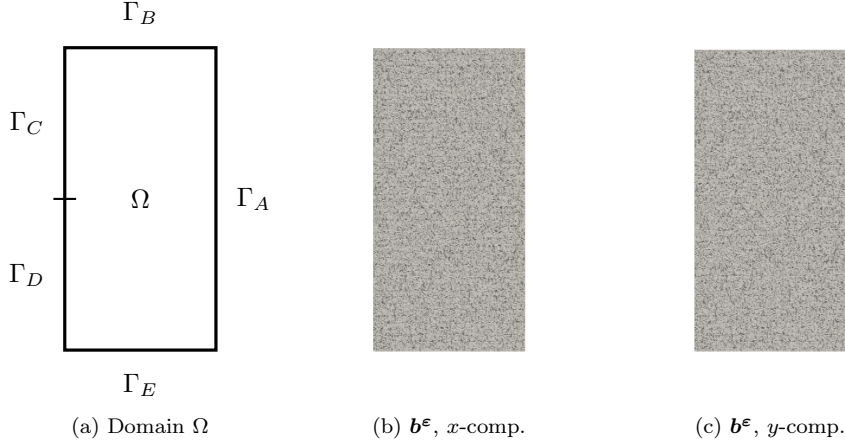


Figure 3: The computational domain Ω for the advection-diffusion test case (a) and the random vector field \mathbf{b}^ϵ (b/c).

A rectangular domain Ω is chosen (see Fig. 3) with homogeneous Dirichlet boundary conditions on Γ_D , homogeneous Neumann conditions on Γ_A , Γ_B and Γ_C , and $\gamma \partial_{\mathbf{n}} u^\epsilon \equiv 1$ on Γ_E . The source term is set to $f \equiv 0$ and the quantity of interest is chosen to be

$$(5.9) \quad \langle j, \varphi \rangle = \int_{\Gamma_B} \varphi \, do_x.$$

In spirit of Definition 2.5, a reduced dual problem with a local enhancement can be defined

$$(5.10) \quad (\bar{A}^\delta \nabla \varphi, \nabla z^\delta) - (\mathbf{b}^\delta \cdot \nabla z^\delta, \varphi) = \langle j, \varphi \rangle \quad \forall \varphi \in V,$$

$$(5.11) \quad \gamma (\nabla \varphi, \nabla (z^\delta + z_K^\delta))_K - ((\mathbf{b}^\epsilon - \mathbf{b}^\delta) \cdot \nabla (z^\delta + z_K^\delta), \varphi)_K = \langle j, \varphi \rangle \quad \forall \varphi \in V(K).$$

Here, the local reconstruction $z_K^\delta \in V(K)$ has homogeneous Dirichlet conditions on *interior* boundary parts ∂K but shall have homogeneous Neumann conditions on all Neumann boundaries of the primal problem, i.e., on boundaries $\partial K \cap \Gamma_i$ with $i = A, B, C, E$. For the choice $\epsilon = 2^{-8}$, $\gamma = 0.1$, as well as values of the advection field with magnitude in the range $0 - 300$, a reference computation with 8.39×10^6 degrees of freedom yields the result $\langle j, u_{\text{ref}}^\epsilon \rangle \approx 0.2170$. A uniform sampling mesh with 32 sampling regions is chosen, as well as a macroscale discretization of 1.3×10^5 cells and a (fully resolved) microscale discretization with $h = 2^{-11}$. The optimization framework is run for a fully resolved dual solution (“full”) with 2.1×10^6 cells as well as the reduced, locally enhanced variant given in Definition 2.5 (“enhanced”). As stopping criterion a reduction of $|\tilde{\theta}^\delta|$ to less than 5% of the initial value is chosen with a penalty $\lambda = 1.0m$, where m is the absolute mean value of the diagonal entries of the matrix $\mathcal{J}^T \mathcal{J}$, see (4.10), and a very small regularization $\alpha_K = 0.1$ (compared to $|\tilde{\theta}^\delta|^2 / |\bar{A}_K^\delta|^2 \sim 1000$). The numerical results are given in Table 2.

To examine the numerical stability of the optimization algorithm the computation is actually run for 15 adaptation cycles well beyond the stopping criterion that

Table 2: Results for the model-optimization algorithm (Algorithm 2) applied to the advection-diffusion problem (5.3) with fully resolved dual solution (a) and for the reduced, locally enhanced variant (b). After steps 12 and 10, respectively, the estimator $|\tilde{\theta}^\delta|$ is reduced to less than 5 % of its initial value.

(a) model-optimization algorithm with fully resolved dual solution						
	$L^2(\Omega)$	$ \langle j, U \rangle $	$ \langle j, u^\varepsilon - U \rangle $	$ \tilde{\theta}^\delta $	I_{eff}	I_{loc}
1	4.43e-1	3.86e-1	-1.69e-1 (77.9 %)	-1.69e-1	1.00	2.21
3	2.80e-1	2.71e-1	-5.36e-2 (24.7 %)	-5.38e-2	1.00	4.24
5	2.29e-1	2.49e-1	-3.16e-2 (14.6 %)	-3.18e-2	1.00	5.86
7	1.90e-1	2.37e-1	-2.02e-2 (9.30 %)	-2.04e-2	1.00	7.68
9	1.60e-1	2.30e-1	-1.32e-2 (6.08 %)	-1.34e-2	1.00	10.2
11	1.39e-1	2.26e-1	-9.14e-3 (4.21 %)	-9.35e-3	1.00	13.2
12	1.30e-1	2.25e-1	-7.91e-3 (3.64 %)	-8.12e-3	1.00	14.7
15	1.13e-1	2.23e-1	-6.28e-3 (2.89 %)	-6.51e-3	0.99	17.3

(b) model-optimization algorithm with reduced, locally enhanced dual solution						
	$L^2(\Omega)$	$ \langle j, U \rangle $	$ \langle j, u^\varepsilon - U \rangle $	$ \tilde{\theta}^\delta $	I_{eff}	I_{loc}
1	4.43e-1	3.86e-1	-1.69e-1 (77.9 %)	-2.96e-1	1.76	2.15
3	2.33e-1	2.62e-1	-4.48e-2 (20.6 %)	-4.92e-2	1.10	4.01
5	1.46e-1	2.39e-1	-2.20e-2 (10.1 %)	-2.85e-2	1.30	3.85
7	9.86e-2	2.28e-1	-1.08e-2 (4.97 %)	-2.06e-2	1.90	3.80
9	8.21e-2	2.22e-1	-5.22e-3 (2.40 %)	-1.58e-2	3.04	4.20
10	7.99e-2	2.20e-1	-3.02e-3 (1.39 %)	-1.27e-2	4.18	4.91
15	9.70e-2	2.14e-1	3.07e-3 (1.41 %)	7.00e-3	2.28	10.4

is reached with step 12 for the full dual solution and with step 10 for the local enhancement strategy. The initial error of 80 % in the target functional with a starting model $\bar{A}_K^\delta = \gamma \text{Id}$ can be reduced to around 2 – 3 % for both variants of dual solution. Further, the adaptation cycle remains stable beyond the point where the stopping criterion was reached. Reference, initial and final (for step 12 and 10, respectively) solutions are depicted in Figure 4. As can be seen from the numerical results, the microscale advection due to \mathbf{b}^ε leads to a locally increased value for \bar{A}_K^δ in the range 0.01 – 0.02 compared to the initial choice $\bar{A}_K^\delta = \gamma \text{Id} \sim 0.01$. The effective models found with the optimization approach match the reference solution quite well near the boundary Γ_B . In contrast, on the far end of Γ_B near the inhomogeneous Neumann condition on Γ_E , the effective solutions deviate from u^ε . This has to be expected as the optimization problem only minimizes the error given by an integral over Γ_B .

6. Conclusion. A novel approach for model adaptivity is proposed that is based on solving an optimization problem by minimizing the local model-error indicators derived from a DWR formulation. The optimization approach allows to derive an efficient post-processing strategy that can be regarded as a multiscale approach in its own right. Its strength lies in the fact that it is in principle independent of strong a priori knowledge about applicability of efficient models—its efficiency is rooted in the almost quantitative behavior of the DWR method when combined with a suitable

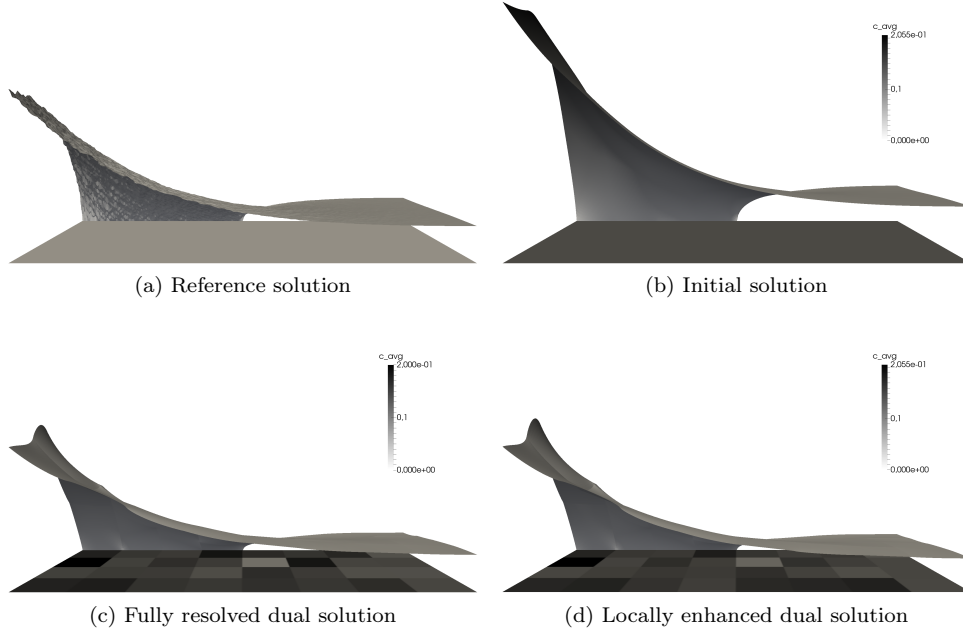


Figure 4: 3 dimensional plot of the reference solution (a), the initial solution $u^{\delta,0}$ of the optimization problem (b), and the solutions of the final models for fully resolved (c) and reduced, locally enhanced (d) dual solution. The figures are a 3 dimensional view from the right side Γ_A onto Ω . The height is given by the value u^ε , $u^{\delta,i}$, the scale is kept the same. Onto Ω itself the values $|\bar{A}^{\delta,i}|$ are plotted.

localization technique for the dual problem. The modeling aspect of the optimization problem lies in the choice of the functional $\langle j, \cdot \rangle$ as quantity of interest (given by the application in mind) and the choice of the localization approach for the dual problem. In this sense it lifts the question of suitable approximation in terms of a quantity of interest (for the primal problem) to the question of suitable approximation properties of the localization technique for the dual problem. The important property here is that the latter is typically measured in the L^2 -norm of the gradient of the error of the dual approximation, for which—depending on the localization approach—strong approximation properties are available. Prototypical numerical results are presented for a heterogeneous elliptic diffusion and an advection-diffusion problem, that indicate that the optimization approach combined with a localization technique that *globally* uses the same effective model as the primal problem and *locally reconstructs* finescale features of the full dual solution does result in an efficient model-adaptation strategy.

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